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# Semiclassical expectation values for relativistic particles with spin $1/2$

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## Abstract

For relativistic particles with spin  $1/2$ , which are described by the Dirac equation, a semiclassical trace formula is introduced that incorporates expectation values of observables in eigenstates of the Dirac-Hamiltonian. Furthermore, the semiclassical limit of an average of expectation values is expressed in terms of a classical average of the corresponding classical observable.

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# 1 Introduction

The three decades that passed since the completion of Gutzwiller's pioneering work on the trace formula [1] (see also [2]) have witnessed a flourishing development of semiclassical methods in connection with trace formulae. Gutzwiller himself, e.g., applied his semiclassical representation of the spectral density in terms of a sum over classical periodic orbits to the quantisation of the anisotropic Kepler problem [1, 3]. Later, in the context of the then developing field of quantum chaos, it was realised that the Gutzwiller trace formula can quite generally be employed for a semiclassical quantisation of classically chaotic systems, where no Bohr-Sommerfeld (or Einstein-Brillouin-Keller) type quantisation is available. A number of semiclassical quantisation schemes were invented and successfully passed various tests, see [2, 4, 5] for collections of examples. On the other hand, Hannay and Ozorio de Almeida [6] and Berry [7] realised that a semiclassical analysis of spectral correlations can be based on trace formulae. These techniques, which have meanwhile been refined in several aspects, still provide the strongest analytic support for the conjectured universality in energy level statistics [8].

Shortly after Gutzwiller established his trace formula, and apparently independently thereof, mathematicians began to prove various versions of semiclassical trace formulae [9, 10, 11, 12, 13]. Moreover, generalisations of the trace formula as a semiclassical representation of the spectral density were developed, e.g., to include also expectation values of observables [14, 12]. Thus, by now the Gutzwiller trace formula is a well developed and well established tool in semiclassical quantum mechanics.

So far, trace formulae have been derived for quantum systems with only translational degrees of freedom. These possess a well defined classical limit and thus semiclassical methods can be applied in a straight forward manner. From a physical point of view, however, spin degrees of freedom are of particular importance. Quantum mechanically a spin  $1/2$  of, say, an electron is described in a two- (i.e. finite-) dimensional Hilbert space, lacking a direct classical counterpart, so that a semiclassical description of quantum systems with coupled translational and spin degrees of freedom is less obvious than in the previous cases. However, the semiclassical formalism that was primarily developed in the mathematical community (see, e.g., [10, 11, 12]) can also be applied to derive a trace formula for Dirac- and Pauli-Hamiltonians [15, 16]. For these, alike in Gutzwiller's original trace formula, the spectral density can be expressed in terms of a sum over classical periodic orbits (of the translational motion). Spin enters through weight factors that depend on a phase derived from a 'classical' spin precessing along the classical periodic orbits.

It is the goal of this paper to develop a semiclassical theory for expectation values of observables in the case of relativistic particles with spin  $1/2$ . To this end we first extend the trace formula [15, 16] for Dirac-Hamiltonians to also include expectation values and then discuss averages of expectation values in eigenstates of the Hamiltonian that correspond to a certain spectral interval. In this way average expectation values and fluctuations thereabout are expressed in terms of classical quantities. The article is organised as follows: In section 2 we recall spectral properties of Dirac-Hamiltonians and represent them as Weyl operators. Bounded observables are then introduced in section 3. Subsequently,

in section 4 the semiclassical description of the time evolution operator in terms of a Van Vleck-Gutzwiller propagator for Dirac-Hamiltonians that was developed in [15, 16] is discussed. Section 5 is then devoted to the derivation of the trace formula for the spectral density weighted by expectation values. Finally, in section 6 we calculate averages of expectation values semiclassically.

## 2 The Dirac-Hamiltonian

In relativistic quantum mechanics a point particle of mass  $m$  and charge  $e$  that is exposed to external electromagnetic fields  $\mathbf{E}$  and  $\mathbf{B}$  is described by the Dirac equation. Here we fix an inertial frame and work with fixed coordinates  $(t, \mathbf{x})$  for Minkowski space-time. We moreover assume that in the given frame the fields are static so that the Dirac equation reads

$$i\hbar \frac{\partial \psi}{\partial t}(t, \mathbf{x}) = \hat{H} \psi(t, \mathbf{x}) , \quad (2.1)$$

with the Dirac-Hamiltonian

$$\hat{H} = c\boldsymbol{\alpha} \cdot \left( \frac{\hbar}{i} \nabla - \frac{e}{c} \mathbf{A}(\mathbf{x}) \right) + mc^2 \beta + e\varphi(\mathbf{x}) , \quad (2.2)$$

where  $\varphi, \mathbf{A}$  are electromagnetic potentials so that  $\mathbf{E}(\mathbf{x}) = -\nabla\varphi(\mathbf{x})$  and  $\mathbf{B}(\mathbf{x}) = \nabla \times \mathbf{A}(\mathbf{x})$ . The Dirac algebra  $\alpha_\mu \alpha_\nu + \alpha_\nu \alpha_\mu = 2\delta_{\mu\nu}$ ,  $\mu, \nu = 0, \dots, 3$ , is realised by the hermitian  $4 \times 4$  matrices

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \quad \text{and} \quad \alpha_0 = \beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix} , \quad (2.3)$$

where  $\sigma_k$ ,  $k = 1, 2, 3$ , are the Pauli matrices and  $\mathbb{1}_n$  denotes the  $n \times n$  unit matrix. For more details see [17].

If the potentials  $\varphi, A_k$  are smooth functions, or at most have Coulomb singularities at some points  $\mathbf{x}_j$  such that

$$|e\varphi(\mathbf{x})|, |eA_k(\mathbf{x})| \leq \frac{a}{|\mathbf{x} - \mathbf{x}_j|} + b \quad (2.4)$$

holds for some constants  $a < \frac{\hbar c}{2}$ ,  $b > 0$  and for all  $\mathbf{x} \in \mathbb{R}^3 \setminus \{\mathbf{x}_j\}$ , the Dirac-Hamiltonian (2.2) is essentially self-adjoint on the domain  $C_0^\infty(\mathbb{R}^3 \setminus \{\mathbf{x}_j\}) \otimes \mathbb{C}^4$  in the Hilbert space  $\mathcal{H} = L^2(\mathbb{R}^3) \otimes \mathbb{C}^4$  of square-integrable Dirac spinors (see, e.g., [17]). The quantum Hamiltonian is then given by the (unique) self-adjoint extension which we also denote by  $\hat{H}$ . As an example consider an electron in the Coulomb potential of a nucleus with charge  $Ze$ , such that  $e\varphi(\mathbf{x}) = -\frac{Ze^2}{|\mathbf{x}|}$ . Since the fine structure constant  $\alpha = \frac{e^2}{\hbar c}$  is approximately given by  $\frac{1}{137}$ , the bound (2.4) implies essential self-adjointness for  $Z \leq 68$ . In the case  $\mathbf{A} = 0$  and  $\varphi$  spherically symmetric, however, the bound on  $a$  can be improved by a factor of  $\sqrt{3}$ ,

leading to  $Z \leq 118$ . For larger  $Z$  one has to choose special self-adjoint extensions, see [17] for further details.

Dirac-Hamiltonians (2.2) possess spectra that are not bounded from below. In fact, if the electromagnetic fields vanish as  $|\mathbf{x}| \rightarrow \infty$ , the essential spectrum of  $\hat{H}$  is given by

$$\sigma_{ess}(\hat{H}) = (-\infty, -mc^2] \cup [mc^2, +\infty) . \quad (2.5)$$

(This is also true under appropriate weaker conditions, see [17].) In what follows we will always consider situations where  $\hat{H}$  is (essentially) self-adjoint and where (2.5) holds. Since below we are only interested in properties of the discrete spectrum of Dirac-Hamiltonians, we will therefore concentrate on the eigenvalues  $E_n$  of  $\hat{H}$  with  $|E_n| < mc^2$ . More precisely, we choose some energy  $E$  in the gap of  $\sigma_{ess}(\hat{H})$  and introduce an interval

$$I(E; \hbar) := [E - \hbar\omega, E + \hbar\omega] , \quad \omega > 0 \text{ fixed} , \quad (2.6)$$

that has no overlap with the essential spectrum of  $\hat{H}$ . This only requires  $\hbar$  to be sufficiently small. We are then interested in the eigenvalues  $E_n \in I(E; \hbar)$  and the expectation values  $\langle \psi_n, \hat{B} \psi_n \rangle$  of observables  $\hat{B}$  in eigenstates  $\psi_n$  related to these eigenvalues.

For the purpose of semiclassical asymptotics it is advantageous to view the Hamiltonian, as well as all further observables, as Weyl operators. For simplicity we now assume that the potentials are smooth so that the Weyl representation

$$(\hat{H}\psi)(\mathbf{x}) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} H\left(\mathbf{p}, \frac{\mathbf{x} + \mathbf{y}}{2}\right) e^{\frac{i}{\hbar}\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \psi(\mathbf{y}) \, d\mathbf{p} \, d\mathbf{y} \quad (2.7)$$

of  $\hat{H}$  holds for  $\psi \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4$ . Here

$$\begin{aligned} H(\mathbf{p}, \mathbf{x}) &:= c\boldsymbol{\alpha} \cdot \left( \mathbf{p} - \frac{e}{c}\mathbf{A}(\mathbf{x}) \right) + mc^2\beta + e\varphi(\mathbf{x}) \\ &= \begin{pmatrix} (e\varphi(\mathbf{x}) + mc^2)\mathbb{1}_2 & (c\mathbf{p} - e\mathbf{A}(\mathbf{x})) \cdot \boldsymbol{\sigma} \\ (c\mathbf{p} - e\mathbf{A}(\mathbf{x})) \cdot \boldsymbol{\sigma} & (e\varphi(\mathbf{x}) - mc^2)\mathbb{1}_2 \end{pmatrix} \end{aligned} \quad (2.8)$$

is the Weyl symbol of  $\hat{H}$ , which for all  $(\mathbf{p}, \mathbf{x}) \in \mathbb{R}^3 \times \mathbb{R}^3$  is a hermitian  $4 \times 4$  matrix with the two twofold degenerate eigenvalues

$$H^\pm(\mathbf{p}, \mathbf{x}) = e\varphi(\mathbf{x}) \pm \sqrt{(c\mathbf{p} - e\mathbf{A}(\mathbf{x}))^2 + m^2c^4} , \quad (2.9)$$

such that  $H^+ - H^- \geq 2mc^2 > 0$ . These eigenvalues are the classical Hamiltonians for relativistic particles (without spin) with positive and negative kinetic energies, respectively, that are exposed to the electromagnetic fields generated by the potentials  $\varphi$  and  $\mathbf{A}$ . The presence of these two eigenvalues is a remnant of the fact that the Dirac equation (2.1) describes both particles and anti-particles, and the dimension of the corresponding eigenspaces follows from the spin 1/2 of the particles and anti-particles, respectively.

One can now introduce an orthonormal basis of  $\mathbb{C}^4$  consisting of the eigenvectors  $e_1(\mathbf{p}, \mathbf{x}), e_2(\mathbf{p}, \mathbf{x})$  of  $H(\mathbf{p}, \mathbf{x})$  with eigenvalue  $H^+(\mathbf{p}, \mathbf{x})$  and the eigenvectors  $f_1(\mathbf{p}, \mathbf{x}), f_2(\mathbf{p}, \mathbf{x})$

with eigenvalue  $H^-(\mathbf{p}, \mathbf{x})$ . This basis allows to construct the  $4 \times 2$  matrices  $V_+(\mathbf{p}, \mathbf{x})$  and  $V_-(\mathbf{p}, \mathbf{x})$  with  $e_1(\mathbf{p}, \mathbf{x})$ ,  $e_2(\mathbf{p}, \mathbf{x})$  and  $f_1(\mathbf{p}, \mathbf{x})$ ,  $f_2(\mathbf{p}, \mathbf{x})$ , respectively, as columns [15, 16],

$$\begin{aligned} V_+(\mathbf{p}, \mathbf{x}) &= \frac{1}{\sqrt{2\varepsilon(\mathbf{p}, \mathbf{x})(\varepsilon(\mathbf{p}, \mathbf{x}) + mc^2)}} \begin{pmatrix} (\varepsilon(\mathbf{p}, \mathbf{x}) + mc^2)\mathbb{1}_2 \\ (c\mathbf{p} - e\mathbf{A}(\mathbf{x})) \cdot \boldsymbol{\sigma} \end{pmatrix}, \\ V_-(\mathbf{p}, \mathbf{x}) &= \frac{1}{\sqrt{2\varepsilon(\mathbf{p}, \mathbf{x})(\varepsilon(\mathbf{p}, \mathbf{x}) + mc^2)}} \begin{pmatrix} (c\mathbf{p} - e\mathbf{A}(\mathbf{x})) \cdot \boldsymbol{\sigma} \\ -(\varepsilon(\mathbf{p}, \mathbf{x}) + mc^2)\mathbb{1}_2 \end{pmatrix}, \end{aligned} \quad (2.10)$$

where

$$\varepsilon(\mathbf{p}, \mathbf{x}) := \sqrt{(c\mathbf{p} - e\mathbf{A}(\mathbf{x}))^2 + m^2c^4}. \quad (2.11)$$

The columns of  $V_\pm$  being orthonormal implies that these matrices represent isometries from  $\mathbb{C}^2$  into  $\mathbb{C}^4$  so that  $V_\pm^\dagger V_\pm = \mathbb{1}_2$ . Moreover, the projectors  $P_0^\pm(\mathbf{p}, \mathbf{x})$  onto the eigenspaces corresponding to the eigenvalues  $H^\pm(\mathbf{p}, \mathbf{x})$  are given by  $P_0^\pm = V_\pm V_\pm^\dagger$ .

### 3 Observables

The kind of observables we are going to consider are given by matrix valued Weyl operators as in (2.7), i.e.

$$(\hat{B}\psi)(\mathbf{x}) = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} B\left(\mathbf{p}, \frac{\mathbf{x} + \mathbf{y}}{2}; \hbar\right) e^{\frac{i}{\hbar}\mathbf{p} \cdot (\mathbf{x} - \mathbf{y})} \psi(\mathbf{y}) \, d\mathbf{p} \, d\mathbf{y}, \quad (3.1)$$

that yield bounded and self-adjoint operators on  $\mathcal{H}$ . Notice that here the symbol  $B(\mathbf{p}, \mathbf{x}; \hbar)$  is allowed to depend on  $\hbar$ . In order to ensure that the operator  $\hat{B}$  defined by (3.1) is bounded one can impose the following condition on its symbol: it shall be smooth in the variables  $(\mathbf{p}, \mathbf{x})$  and, moreover, possess an asymptotic expansion

$$B(\mathbf{p}, \mathbf{x}; \hbar) \sim \sum_{j \geq 0} \hbar^j B_j(\mathbf{p}, \mathbf{x}) \quad (3.2)$$

in the sense that for all  $N \geq 0$  and all multi-indices  $\alpha, \beta \in \mathbb{N}_0^3$

$$\left\| \partial_p^\alpha \partial_x^\beta \left( B(\mathbf{p}, \mathbf{x}; \hbar) - \sum_{j=0}^N \hbar^j B_j(\mathbf{p}, \mathbf{x}) \right) \right\|_{4 \times 4} \leq C_{\alpha\beta} \hbar^{N+1}. \quad (3.3)$$

In particular,  $B$  and all of its derivatives shall be bounded. Here  $\|\dots\|_{4 \times 4}$  denotes an arbitrary matrix norm and the short-hand  $\partial_x^\alpha = \frac{\partial^{\alpha_1 + \alpha_2 + \alpha_3}}{\partial x_1^{\alpha_1} \partial x_2^{\alpha_2} \partial x_3^{\alpha_3}}$  has been used. The leading term  $B_0(\mathbf{p}, \mathbf{x})$  in the semiclassical asymptotics (3.2) is called *principal symbol* and will be viewed as the classical observable corresponding to the quantum observable  $\hat{B}$ . For scalar symbols a proof for the fact that (3.3) implies the boundedness of  $\hat{B}$  can, e.g., be found in [18]; this immediately carries over to the present situation, see also [19]. The operator

$\hat{B}$  defined by (3.1) for  $\psi \in C_0^\infty(\mathbb{R}^3) \otimes \mathbb{C}^4$  hence can now be extended to all of  $\mathcal{H}$  and is self-adjoint as soon as its symbol  $B(\mathbf{p}, \mathbf{x}; \hbar)$  is hermitian. In the following we will always assume this to be the case.

Two particular classical observables are the projectors  $P_0^\pm(\mathbf{p}, \mathbf{x})$  onto the eigenspaces of the symbol (2.8) of the Dirac-Hamiltonian. If we assume that the potentials and all of their derivatives are bounded, which poses no severe restriction since we want the electromagnetic fields to vanish as  $|\mathbf{x}| \rightarrow \infty$ , an inspection of (2.10) reveals that  $P_0^\pm(\mathbf{p}, \mathbf{x})$  together with all derivatives are also bounded. A Weyl quantisation of  $P_0^\pm(\mathbf{p}, \mathbf{x})$  hence yields bounded operators  $\hat{P}_0^\pm$ . These, however, are not yet projection operators on  $\mathcal{H}$ , but a semiclassical construction, see [20, 21], allows to introduce bounded and self-adjoint operators  $\hat{P}^\pm$  with principal symbols  $P_0^\pm(\mathbf{p}, \mathbf{x})$  that obey  $\hat{P}^+ + \hat{P}^- = \mathbb{1}_{\mathcal{H}}$ . Moreover, up to terms of order  $\hbar^\infty$  these operators fulfill  $(\hat{P}^\pm)^2 = \hat{P}^\pm$ ,  $\hat{P}^+ \hat{P}^- = 0$  and commute with  $\hat{H}$ . With respect to these semiclassical projectors one can now split an observable  $\hat{B}$  of the type introduced above according to

$$\hat{B} = \hat{B}_d + \hat{B}_{nd} , \quad (3.4)$$

where

$$\hat{B}_d := \hat{P}^+ \hat{B} \hat{P}^+ + \hat{P}^- \hat{B} \hat{P}^- \quad \text{and} \quad \hat{B}_{nd} := \hat{P}^+ \hat{B} \hat{P}^- + \hat{P}^- \hat{B} \hat{P}^+ \quad (3.5)$$

denote the diagonal and the non-diagonal part, respectively. According to the product rule for Weyl operators (see, e.g., [22, 18])  $\hat{B}_d$  and  $\hat{B}_{nd}$  are again bounded and self-adjoint Weyl operators with principal symbols

$$\begin{aligned} B_{d,0}(\mathbf{p}, \mathbf{x}) &= P_0^+(\mathbf{p}, \mathbf{x}) B_0(\mathbf{p}, \mathbf{x}) P_0^+(\mathbf{p}, \mathbf{x}) + P_0^-(\mathbf{p}, \mathbf{x}) B_0(\mathbf{p}, \mathbf{x}) P_0^-(\mathbf{p}, \mathbf{x}) , \\ B_{nd,0}(\mathbf{p}, \mathbf{x}) &= P_0^+(\mathbf{p}, \mathbf{x}) B_0(\mathbf{p}, \mathbf{x}) P_0^-(\mathbf{p}, \mathbf{x}) + P_0^-(\mathbf{p}, \mathbf{x}) B_0(\mathbf{p}, \mathbf{x}) P_0^+(\mathbf{p}, \mathbf{x}) . \end{aligned} \quad (3.6)$$

## 4 Semiclassical time evolution

In this section we mainly review the derivation of the Van Vleck-Gutzwiller propagator for Dirac-Hamiltonians that was developed in [15, 16]. For a detailed exposition see [16]. The aim here is to obtain the semiclassically leading asymptotics of the Schwartz kernel  $K(\mathbf{x}, \mathbf{y}, t)$  for the unitary time evolution operator  $\hat{U}(t) = e^{-\frac{i}{\hbar} t \hat{H}}$ . Given an initial state  $\psi_0 \in \mathcal{H}$ , the solution  $\psi(t) = \hat{U}(t) \psi_0$  of the Dirac equation (2.1) with initial condition  $\psi(0) = \psi_0$  reads in coordinate representation

$$\psi(t, \mathbf{x}) = \int_{\mathbb{R}^3} K(\mathbf{x}, \mathbf{y}, t) \psi_0(\mathbf{y}) \, d\mathbf{y} , \quad (4.1)$$

so that the initial condition for the kernel is  $K(\mathbf{x}, \mathbf{y}, 0) = \delta(\mathbf{x} - \mathbf{y})$ . Up to terms of order  $\hbar^\infty$  this kernel can be approximated by a semiclassical Fourier integral operator, i.e.

$$\begin{aligned} K(\mathbf{x}, \mathbf{y}, t) &= \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} \left[ a_h^+(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}) e^{\frac{i}{\hbar} \phi^+(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi})} \right. \\ &\quad \left. + a_h^-(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}) e^{\frac{i}{\hbar} \phi^-(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi})} \right] d\boldsymbol{\xi} + O(\hbar^\infty) . \end{aligned} \quad (4.2)$$

The two additive contributions under the integral refer to the two eigenvalues  $H^\pm$  of the symbol  $H$  of the Dirac-Hamiltonian, which each serve as a classical Hamiltonian. The amplitude factors  $a_h^\pm$  take values in the  $4 \times 4$  matrices and are assumed to allow for the asymptotic expansions

$$a_h^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}) = \sum_{k \geq 0} \left(\frac{\hbar}{i}\right)^k a_k^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}) , \quad (4.3)$$

with initial conditions

$$a_k^\pm(\mathbf{x}, \mathbf{y}, 0, \boldsymbol{\xi}) = \begin{cases} P_0^\pm(\boldsymbol{\xi}, \mathbf{x}) & \text{if } k = 0 , \\ 0 & \text{if } k \geq 1 . \end{cases} \quad (4.4)$$

Together with the initial condition  $\phi^\pm|_{t=0} = \boldsymbol{\xi} \cdot (\mathbf{x} - \mathbf{y})$  for the phase function this ensures the desired behaviour of the representation (4.2) for  $t \rightarrow 0$ .

The strategy to obtain a semiclassical approximation for  $K(\mathbf{x}, \mathbf{y}, t)$  now is the same as in the WKB method: one inserts the ansatz (4.2) with the expansion (4.3) into the Dirac equation, groups terms together with like powers of  $\hbar$ , and equates these terms to zero. This yields a hierarchy of equations for the phase functions  $\phi^\pm$  and the coefficients  $a_k^\pm$  that have to be solved order by order in  $k$ . The lowest order ( $k = 0$ ) equation, together with the definition  $S^\pm(\boldsymbol{\xi}, \mathbf{x}, t) := \phi^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}) + \boldsymbol{\xi} \cdot \mathbf{y}$ , relates the phase functions  $\phi^\pm$  to the solutions  $S^\pm$  of the associated Hamilton-Jacobi equations

$$H^\pm(\nabla_x S^\pm(\boldsymbol{\xi}, \mathbf{x}, t), \mathbf{x}) + \frac{\partial S^\pm}{\partial t}(\boldsymbol{\xi}, \mathbf{x}, t) = 0 \quad \text{with} \quad S^\pm(\boldsymbol{\xi}, \mathbf{x}, 0) = \boldsymbol{\xi} \cdot \mathbf{x} . \quad (4.5)$$

Hence  $S^\pm$  generate canonical transformations  $(\mathbf{p}^\pm, \mathbf{x}) \mapsto (\boldsymbol{\xi}, \mathbf{z}^\pm)$  with  $\mathbf{p}^\pm = \nabla_x S^\pm(\boldsymbol{\xi}, \mathbf{x}, t)$  and  $\mathbf{z}^\pm = \nabla_\xi S^\pm(\boldsymbol{\xi}, \mathbf{x}, t)$  such that  $(\boldsymbol{\xi}, \mathbf{z}^\pm)$  and  $(\mathbf{p}^\pm, \mathbf{x})$  are starting and end points, respectively, of solutions  $(\mathbf{P}^\pm(t'), \mathbf{X}^\pm(t'))$ ,  $0 \leq t' \leq t$ , of the classical equations of motion generated by  $H^\pm$ .

The leading semiclassical asymptotics for the amplitudes then follows from both the equations in leading and next-to-lowest order. For sufficiently small  $t$  the result reads

$$a_0^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}) = \sqrt{\det\left(\frac{\partial^2 S^\pm}{\partial \xi \partial x}(\boldsymbol{\xi}, \mathbf{x}, t)\right)} \quad (4.6)$$

$$V_\pm(\nabla_x S^\pm(\boldsymbol{\xi}, \mathbf{x}, t), \mathbf{x}) \tilde{d}_\pm(\nabla_x S^\pm(\boldsymbol{\xi}, \mathbf{x}, t), \mathbf{x}) V_\pm^\dagger(\boldsymbol{\xi}, \mathbf{y}) .$$

The restriction to small  $t$  stems from the non-uniqueness of the solutions  $S^\pm$  of the Hamilton-Jacobi equations (4.5) for times beyond which caustics appear. One is, however, faced with the same problem already in the context of non-relativistic, spinless particles where the respective solution merely consists of the first factor on the right-hand side of (4.6). For this case Gutzwiller showed [23] that one can pass beyond caustics with a correct choice of the phase in the first term of (4.6) when sign changes occur under the square-root. The appropriate phase factor that Gutzwiller introduced essentially consists of the Morse

index of the related classical trajectory. A mathematically rigorous justification of this construction can, e.g., be found in [10, 11]. Obviously, exactly the same procedure can be applied to extend (4.6) to arbitrary, however finite, times.

The factor  $\tilde{d}_\pm$  appearing in (4.6) is a solution of the spin transport equation

$$\left(\frac{d}{dt} + iM_\pm(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t))\right) \tilde{d}_\pm(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t)) = 0, \quad (4.7)$$

with initial condition  $\tilde{d}_\pm(\mathbf{P}^\pm(0), \mathbf{X}^\pm(0)) = \mathbb{1}_2$ , in which the time derivative is to be taken along the solutions  $(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t))$  of the classical equations of motion that are generated by the solutions  $S^\pm$  of the Hamilton-Jacobi equations (4.5). The  $2 \times 2$  matrices

$$M_\pm(\mathbf{p}, \mathbf{x}) := \mp \frac{ec}{2\varepsilon(\mathbf{p}, \mathbf{x})} \left[ \mathbf{B}(\mathbf{x}) \pm \frac{c}{\varepsilon(\mathbf{p}, \mathbf{x}) + mc^2} \left( \mathbf{E}(\mathbf{x}) \times \left( \mathbf{p} - \frac{e}{c} \mathbf{A}(\mathbf{x}) \right) \right) \right] \cdot \boldsymbol{\sigma} \quad (4.8)$$

are hermitian and traceless so that according to (4.7) the spin transport matrices  $\tilde{d}_\pm$  take values in  $SU(2)$ . Since the solutions  $(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t))$  of Hamilton's equations of motion depend on the initial points  $(\boldsymbol{\xi}, \mathbf{z}^\pm)$ , below we also write  $d_\pm(\boldsymbol{\xi}, \mathbf{z}^\pm, t)$  for  $\tilde{d}_\pm(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t))$ . In these variables the composition law of the spin transport matrices reads

$$d_\pm(\boldsymbol{\xi}, \mathbf{z}^\pm, t + t') = d_\pm(\mathbf{P}^\pm(t'), \mathbf{X}^\pm(t'), t) d_\pm(\boldsymbol{\xi}, \mathbf{z}^\pm, t'). \quad (4.9)$$

In order to calculate the leading semiclassical asymptotics of the time evolution kernel  $K(\mathbf{x}, \mathbf{y}, t)$  further one employs the method of stationary phase to the integral (4.2). Due to the connection of the phases  $\phi^\pm$  with the solutions  $S^\pm$  of the Hamilton-Jacobi equations, the stationary points  $\boldsymbol{\xi}_{st}$  of  $\phi^\pm$  are such that the canonical transformations generated by  $S^\pm(\boldsymbol{\xi}_{st}, \mathbf{x}, t)$  map  $(\mathbf{p}^\pm, \mathbf{x})$  to  $(\boldsymbol{\xi}_{st}, \mathbf{y})$ . These are therefore the end and starting points, respectively, of the associated solutions  $(\mathbf{P}^\pm(t'), \mathbf{X}^\pm(t'))$  of the equations of motion. Thus the stationary points  $\boldsymbol{\xi}_{st}$  are in one-to-one correspondence with the classical trajectories  $\gamma^\pm$  connecting  $\mathbf{y}$  to  $\mathbf{x}$  in time  $t$ . The expression that finally results from the application of the method of stationary phase is to a large extent analogous to the Van Vleck-Gutzwiller propagator (see [23]) for non-relativistic, spinless particles. Differences arise due to (i) the presence of two kinds of classical dynamics (generated by the two Hamiltonians  $H^\pm$ ) instead of one, and (ii) the presence of the additional factors in the amplitude (4.6). The latter, however, need only be evaluated at the stationary points  $\boldsymbol{\xi}_{st}$ . As a result one therefore obtains

$$K(\mathbf{x}, \mathbf{y}, t) = \frac{1}{(2\pi i \hbar)^{3/2}} \sum_{\gamma^\pm} V_\pm(t) d_\pm V_\pm^\dagger(0) D_{\gamma^\pm} e^{\frac{i}{\hbar} R_{\gamma^\pm}^\pm - i \frac{\pi}{2} \nu_{\gamma^\pm}} (1 + O(\hbar)). \quad (4.10)$$

Here the sum extends over all solutions  $\gamma^\pm$  of the equations of motion from  $\mathbf{y}$  to  $\mathbf{x}$  in time  $t$ , and  $\nu_{\gamma^\pm}$  denotes their Morse indices. Moreover, the phase functions  $\phi^\pm$  evaluated at the stationary point  $\boldsymbol{\xi}_{st}$  related to  $\gamma^\pm$  turn out to be Hamilton's principal functions  $R_{\gamma^\pm}^\pm(\mathbf{x}, \mathbf{y}, t) = S^\pm(\boldsymbol{\xi}_{st}, \mathbf{x}, t) - \boldsymbol{\xi}_{st} \cdot \mathbf{y}$ , and

$$D_{\gamma^\pm} := \left| \det \left( -\frac{\partial^2 R_{\gamma^\pm}^\pm}{\partial x \partial y}(\mathbf{x}, \mathbf{y}, t) \right) \right|^{1/2}. \quad (4.11)$$



We also introduced the abbreviation  $V_{\pm}(t') := V_{\pm}(\mathbf{P}^{\pm}(t'), \mathbf{X}^{\pm}(t'))$ .

Inspecting (4.10) reveals a close similarity to the Van Vleck-Gutzwiller propagator. The summation goes over the classical trajectories of relativistic particles, such that here only the translational dynamics is relevant. The spin dynamics then enters through the additional factor  $V_{\pm}(t) d_{\pm} V_{\pm}^{\dagger}(0)$  that describes the precession of a two-component spinor along the trajectory  $\gamma^{\pm}$  in the given external fields  $\mathbf{E}$  and  $\mathbf{B}$ . In order to see this recall that  $V_{\pm}^{\dagger}(\mathbf{p}, \mathbf{x})$ , being an isometry from a subspace in  $\mathbb{C}^4$  to  $\mathbb{C}^2$ , projects four-component (Dirac) spinors to two-component spinors. These two components are the expansion coefficients of the projection to the eigenspace  $P_0^{\pm}(\mathbf{p}, \mathbf{x})\mathbb{C}^4$  in the basis  $\{e_1(\mathbf{p}, \mathbf{x}), e_2(\mathbf{p}, \mathbf{x})\}$  or  $\{f_1(\mathbf{p}, \mathbf{x}), f_2(\mathbf{p}, \mathbf{x})\}$ , respectively. The  $SU(2)$  matrix  $d_{\pm}$  then propagates the two-component spinor along the trajectory  $\gamma^{\pm}$  towards its end point. The propagated two-component spinor is then converted back into a four-component (Dirac) spinor by  $V_{\pm}(t)$ . One can thus view the combined dynamics of the spin and translational degrees of freedom as it enters the semiclassical propagator (4.10) to be of a mixed quantum-classical type: the translational dynamics are classical and drive the quantum mechanical spin dynamics. However, it can be shown that expectation values of the spin operator, which is proportional to  $\boldsymbol{\sigma}$ , in the two-component spinors exhibit the well known Thomas precession of a ‘classical’ spin along  $\gamma^{\pm}$ , see [24, 16, 25] for more details. Moreover, knowing the classical spin precession, one can recover the full spin dynamics, as described by the spin transport matrices  $d_{\pm}$ , with the help of a certain dynamical and geometric phase [16].

## 5 The trace formula with expectation values

Having the semiclassical propagator (4.10) available, one could now proceed to derive a semiclassical trace formula, very much in analogy to Gutzwiller’s original trace formula for non-relativistic, spinless particles [1, 2]. One only has to localise in energy first, in order to project out the essential spectrum of the Dirac-Hamiltonian. To this end one chooses a smooth function  $\chi \in C_0^{\infty}(\mathbb{R})$  that is supported in the interval  $(-mc^2, +mc^2)$  where the eigenvalues of  $\hat{H}$  are located that one is interested in. Then  $\chi(\hat{H})$ , defined by the functional calculus given by the spectral theorem, is a bounded and self-adjoint operator with pure point spectrum located in  $\text{supp } \chi$ ; its eigenvalues are  $\chi(E_n)$ . Hence the truncated time evolution operator  $\hat{U}_{\chi}(t) := e^{-\frac{i}{\hbar}t\hat{H}} \chi(\hat{H})$  has a Schwartz kernel with spectral representation

$$K_{\chi}(\mathbf{x}, \mathbf{y}, t) = \sum_n \chi(E_n) \psi_n(\mathbf{x}) \psi_n^{\dagger}(\mathbf{y}) e^{-\frac{i}{\hbar}E_n t} \quad (5.1)$$

in terms of eigenspinors  $\psi_n$  and eigenvalues  $E_n \in \text{supp } \chi$  of  $\hat{H}$ . Since  $K_{\chi}(\mathbf{x}, \mathbf{y}, t) = \chi(\hat{H}) K(\mathbf{x}, \mathbf{y}, t)$ , where  $\chi(\hat{H})$  acts on the variable  $\mathbf{x}$ , the leading semiclassical asymptotics of  $K_{\chi}$  can immediately be concluded from (4.10). The only modification is provided by an additional factor of  $\chi(E_{\gamma^{\pm}})$ , where  $E_{\gamma^{\pm}}$  denotes the energy of the trajectory  $\gamma^{\pm}$ . The result can then be used to derive a semiclassical trace formula; see [15, 16], where this procedure has been carried out.

Here, however, our aim is to include the expectation values  $\langle \psi_n, \hat{B} \psi_n \rangle$  of observables  $\hat{B}$  as they have been introduced in section 3. To this end one considers a suitably regularised trace of the operator  $\hat{B} \hat{U}_\chi(t)$ . The regularisation requires a test function  $\rho \in C^\infty(\mathbb{R})$  with compactly supported Fourier transform,  $\tilde{\rho} \in C_0^\infty(\mathbb{R})$ , so that

$$\hat{U}_\chi[\tilde{\rho}] := \frac{1}{2\pi} \int_{\mathbb{R}} \tilde{\rho}(t) \hat{U}_\chi(t) dt \quad (5.2)$$

defines a bounded operator. The map  $\tilde{\rho} \mapsto \text{Tr} \hat{U}_\chi[\tilde{\rho}]$ , where  $\text{Tr}(\cdot)$  is the operator trace on  $\mathcal{H}$ , then yields a tempered distribution, if the sum  $\sum_n \chi(E_n) \rho(E_n/\hbar)$  is absolutely convergent. The latter condition certainly holds when the eigenvalues do not accumulate in  $\text{supp } \chi$ . One hence should choose  $\chi$  in such a way that possible accumulation points of eigenvalues lie outside of  $\text{supp } \chi$ , and that  $\chi$  vanishes sufficiently fast towards accumulation points. Under this condition one can calculate the trace of the operator  $\hat{B} \hat{U}_\chi[\tilde{\rho} e^{\frac{i}{\hbar} E(\cdot)}]$ ,

$$\text{Tr} \frac{1}{2\pi} \int_{\mathbb{R}} \tilde{\rho}(t) e^{\frac{i}{\hbar} Et} \hat{B} \hat{U}_\chi(t) dt = \sum_n \chi(E_n) \langle \psi_n, \hat{B} \psi_n \rangle \rho\left(\frac{E_n - E}{\hbar}\right). \quad (5.3)$$

The right-hand side of (5.3) already provides the spectral side of the trace formula we are aiming at. The semiclassical side of this trace formula can then be obtained from the left-hand side upon introducing the kernel  $K_\chi$  for  $\hat{U}_\chi$  and calculating the trace in coordinate representation.

Before one can perform this computation, however, one needs the Schwartz kernel for the operator  $\hat{B} \hat{U}_\chi(t)$ , or at least a semiclassical expression for it. The latter can be derived from the representation (4.2) of the time evolution kernel, when one employs the action of a Weyl operator  $\hat{D}$  with symbol  $D(\mathbf{p}, \mathbf{x})$  on functions of the form  $a(\mathbf{x}) e^{\frac{i}{\hbar} \phi(\mathbf{x})}$ . This reads

$$(\hat{D} a e^{\frac{i}{\hbar} \phi})(\mathbf{x}) = (D(\nabla \phi(\mathbf{x}), \mathbf{x}) a(\mathbf{x}) + O(\hbar)) e^{\frac{i}{\hbar} \phi(\mathbf{x})}, \quad (5.4)$$

see, e.g., [26]. In a first step one therefore has to apply the operator  $\hat{D} = \chi(\hat{H})$  to  $K(\mathbf{x}, \mathbf{y}, t)$ , which can be done with the help of (5.4) since according to the functional calculus of [22]  $\chi(\hat{H})$  is a Weyl operator with principal symbol  $D_0(\mathbf{p}, \mathbf{x}) = \chi(H(\mathbf{p}, \mathbf{x}))$ . Then, in a second step, one repeats the procedure with the observable  $\hat{B}$ . Thus

$$\begin{aligned} \hat{B} \chi(\hat{H}) a_0^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}) e^{\frac{i}{\hbar} \phi^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi})} \\ = B_0(\nabla_x \phi^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}), \mathbf{x}) \chi(H^\pm(\nabla_x \phi^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}), \mathbf{x})) \\ a_0^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi}) e^{\frac{i}{\hbar} \phi^\pm(\mathbf{x}, \mathbf{y}, t, \boldsymbol{\xi})} + O(\hbar) \end{aligned} \quad (5.5)$$

yields the leading semiclassical asymptotics for the integrand of the Schwartz kernel for the operator  $\hat{B} \hat{U}_\chi(t)$  in an analogous representation to (4.2). Calculating the trace on the left-hand side of (5.3) in coordinate representation therefore requires, in leading semiclassical order, to evaluate the integrals

$$\begin{aligned} \int_{\mathbb{R}} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \text{tr}(B_0(\nabla_x \phi^\pm, \mathbf{x}) a_0^\pm(\mathbf{x}, \mathbf{x}, t, \boldsymbol{\xi})) \\ \tilde{\rho}(t) \chi(H^\pm(\nabla_x \phi^\pm, \mathbf{x})) e^{\frac{i}{\hbar} (\phi^\pm(\mathbf{x}, \mathbf{x}, t, \boldsymbol{\xi}) + Et)} d\boldsymbol{\xi} dx dt, \end{aligned} \quad (5.6)$$

where  $\text{tr}(\cdot)$  denotes a matrix trace.

Since the integration cannot be performed in closed form, one employs the method of stationary phase. The connection of the phase with the generating functions  $S^\pm$  then reveals that stationary points  $(\boldsymbol{\xi}_{st}, \boldsymbol{x}_{st}, t_{st})$  are such that  $(\boldsymbol{\xi}_{st}, \boldsymbol{x}_{st})$  lies on a periodic orbit  $\gamma_p^\pm$  with energy  $E$  and period  $t_{st}$  of the classical dynamics generated by  $H^\pm$ . One therefore concludes that up to terms of order  $\hbar^\infty$  the expression (5.3) is given by a sum over the periodic orbits  $\gamma_p^\pm$  with periods  $T_{\gamma_p^\pm} \in \text{supp } \tilde{\rho}$ . We recall that the method of stationary phase also demands that at stationary points the phase be non-degenerate. Here this means that transversal to the (connected) manifolds of stationary points, which are at least one dimensional, the matrix of second derivatives of the phase with respect to  $(\boldsymbol{\xi}, \boldsymbol{x}, t)$  must have a (constant) rank of seven minus the dimension of the respective manifold. Let us explicitly mention two examples:

1. The entire hyper-surfaces

$$\Omega_E^\pm := \{(\boldsymbol{p}, \boldsymbol{x}); H^\pm(\boldsymbol{p}, \boldsymbol{x}) = E\} \quad (5.7)$$

of constant energy are manifolds of periodic points with trivial periods  $t_{st} = 0$ . Thus  $\Omega_E^\pm \times \{t_{st} = 0\}$  are five dimensional manifolds of stationary points. In this case the non-degeneracy condition means that  $E$  is a regular value for the Hamiltonians  $H^\pm$ , i.e.  $(\nabla_p H^\pm(\boldsymbol{p}, \boldsymbol{x}), \nabla_x H^\pm(\boldsymbol{p}, \boldsymbol{x})) \neq 0$  for all  $(\boldsymbol{p}, \boldsymbol{x}) \in \Omega_E^\pm$ .

2. An isolated periodic orbit  $\gamma_p^\pm$  is non-degenerate, if its monodromy matrix  $\mathbb{M}_{\gamma_p^\pm}$ , i.e. the restriction of the linearised Poincaré map to the directions transversal to the orbit, has no eigenvalue one.

For simplicity, below we will always restrict attention to these cases, i.e. we require  $E$  to be a regular value for the Hamiltonians and assume that all periodic orbits with energy  $E$  are isolated and non-degenerate. The latter condition is, e.g., fulfilled by hyperbolic periodic orbits, where all eigenvalues of  $\mathbb{M}_{\gamma_p^\pm}$  are different from one in modulus. However, we would like to stress that a semiclassical trace formula can be derived under more general conditions. One only needs a non-degeneracy condition for the manifolds of stationary points in order to be able to apply the method of stationary phase.

For the explicit computation of the semiclassical side of the trace formula one should treat each connected manifold of stationary points separately. To this end we now introduce the partition of unity  $\sum_j h_j(t) = 1$ , with  $h_j \in C_0^\infty(\mathbb{R})$ , under the integral (5.6) such that  $\text{supp } h_j$  contains only one period  $T_{\gamma_p^\pm}$  of a periodic orbit  $\gamma_p^\pm$  with energy  $E$ ; in particular,  $h(T_{\gamma_p^\pm}) = 1$ . Then each summand, labeled by  $j$ , corresponds to a contribution of exactly one (isolated and non-degenerate) periodic orbit. We, furthermore, reserve the label  $j = 0$  for the contribution of the manifolds  $\Omega_E^\pm$  for which  $t_{st} = 0$ . The necessary computations are almost identical to the case of the trace formula without expectation values of an observable and thus we can direct the reader to [16] for the details.

It turns out that the leading semiclassical order of the Weyl term, i.e. of the contribution

with  $j = 0$ , reads

$$\chi(E) \frac{\tilde{\rho}(0)}{2\pi} \frac{1}{(2\pi\hbar)^2} \left[ \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \text{tr}(B_0(\mathbf{p}, \mathbf{x}) P_0^+(\mathbf{p}, \mathbf{x})) \delta(H^+(\mathbf{p}, \mathbf{x}) - E) \, dp \, dx \right. \\ \left. + \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \text{tr}(B_0(\mathbf{p}, \mathbf{x}) P_0^-(\mathbf{p}, \mathbf{x})) \delta(H^-(\mathbf{p}, \mathbf{x}) - E) \, dp \, dx \right] . \quad (5.8)$$

Introducing the notation

$$d\mu_E^\pm(\mathbf{p}, \mathbf{x}) := \frac{1}{\text{vol}(\Omega_E^\pm)} \delta(H^\pm(\mathbf{p}, \mathbf{x}) - E) \, dp \, dx \quad (5.9)$$

for Liouville measure on  $\Omega_E^\pm$ , the leading order of the Weyl term can also be given as

$$\chi(E) \frac{\tilde{\rho}(0)}{2\pi} \frac{1}{(2\pi\hbar)^2} \left[ \text{vol}(\Omega_E^+) \int_{\Omega_E^+} \text{tr}(B_0 P_0^+) \, d\mu_E^+ + \text{vol}(\Omega_E^-) \int_{\Omega_E^-} \text{tr}(B_0 P_0^-) \, d\mu_E^- \right] . \quad (5.10)$$

Since the matrices  $P_0^\pm$  are projectors, the integrands in (5.10) also read  $\text{tr}(B_0 P_0^\pm) = \text{tr}(P_0^\pm B_0 P_0^\pm) =: \text{tr} B_0^\pm$ , and as a short-hand we will also use  $\text{tr} \overline{B_0^\pm}^E$  for the integrals over  $\Omega_E^\pm$ .

In the case of an isolated and non-degenerate periodic orbit  $\gamma_p^\pm$  the evaluation of its contribution to the semiclassical side of the trace formula also proceeds in close analogy to the case without an observable, until it comes to the point where an integration over the primitive periodic orbit associated with  $\gamma_p^\pm$  is required. In the present situation the object that has to be integrated along the primitive orbit is the matrix trace of

$$B_0(\mathbf{p}, \mathbf{x}) V_\pm(\mathbf{p}, \mathbf{x}) d_\pm(\mathbf{p}, \mathbf{x}, T_{\gamma_p^\pm}) V_\pm^\dagger(\mathbf{p}, \mathbf{x}) , \quad (5.11)$$

where the last three factors derive from the spin contribution to the semiclassical propagator (4.10). For the integration we parametrise the periodic orbit by  $(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t))$ ,  $0 \leq t \leq T_{\gamma_p^\pm}^\#$ , where  $T_{\gamma_p^\pm}^\#$  denotes the primitive period associated with  $\gamma_p^\pm$ , and hence have to evaluate (5.11) at  $(\mathbf{p}, \mathbf{x}) = (\mathbf{P}^\pm(t), \mathbf{X}^\pm(t))$ . The quantity that finally enters the trace formula then is a particular average of the principal symbol  $B_0$  of the observable along the primitive periodic orbit,

$$\text{tr} \overline{B_0}^{\gamma_p^\pm} := \frac{1}{T_{\gamma_p^\pm}^\#} \int_0^{T_{\gamma_p^\pm}^\#} \text{tr} \left[ B_0(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t)) V_\pm(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t)) \right. \\ \left. d_\pm(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t), T_{\gamma_p^\pm}) V_\pm^\dagger(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t)) \right] dt . \quad (5.12)$$

The integrand appearing in (5.12) can be interpreted as follows: the right-most term projects a four-component (Dirac) spinor at  $(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t))$  to the local  $H^\pm$ -eigenspace  $P_0^\pm(\mathbf{P}^\pm(t), \mathbf{X}^\pm(t))\mathbb{C}^4$  in a two-component representation. This two-spinor is then propagated once around the periodic orbit and subsequently converted back to a Dirac spinor

which is finally mapped by  $B_0$ . The integration then averages the result of this procedure over the primitive orbit related to  $\gamma_p^\pm$ .

Altogether, if all periodic orbits generated by the two Hamiltonians  $H^\pm$  with an energy  $E$  that is not a critical value for these Hamiltonians are isolated and non-degenerate, the semiclassical trace formula we have been aiming at reads

$$\begin{aligned} \sum_n \chi(E_n) \langle \psi_n, \hat{B} \psi_n \rangle \rho\left(\frac{E_n - E}{\hbar}\right) \\ = \chi(E) \frac{\tilde{\rho}(0)}{2\pi} \frac{1}{(2\pi\hbar)^2} \left( \text{vol}(\Omega_E^+) \text{tr} \overline{B_0^+}^E + \text{vol}(\Omega_E^-) \text{tr} \overline{B_0^-}^E \right) + O(\hbar^{-1}) \\ + \sum_{\gamma_p^\pm} \chi(E) \frac{\tilde{\rho}(T_{\gamma_p^\pm})}{2\pi} \text{tr} \overline{B_0}^{\gamma_p^\pm} A_{\gamma_p^\pm} e^{\frac{i}{\hbar} S_{\gamma_p^\pm}(E)} (1 + O(\hbar)) , \end{aligned} \quad (5.13)$$

where as usual the action of a periodic orbit is denoted as

$$S_{\gamma_p^\pm}(E) := \int_{\gamma_p^\pm} \mathbf{p} \cdot d\mathbf{x} , \quad (5.14)$$

and the amplitude associated with a periodic orbit,

$$A_{\gamma_p^\pm} := \frac{T_{\gamma_p^\pm}^\# e^{-i\frac{\pi}{2}\mu_{\gamma_p^\pm}}}{|\det(\mathbb{M}_{\gamma_p^\pm} - \mathbb{1}_4)|^{1/2}} , \quad (5.15)$$

incorporates the monodromy matrix  $\mathbb{M}_{\gamma_p^\pm}$  and the Maslov index  $\mu_{\gamma_p^\pm}$  of that orbit.

Let us remark that this trace formula reduces to the one derived in [15, 16] in the case  $\hat{B} = \mathbb{1}_{\mathcal{H}}$ . Obviously, on the left-hand side of (5.13) the expectation value then disappears and in the Weyl term  $\text{tr} \overline{B_0^\pm}^E = 2$ . In order to see what happens to the weights  $\text{tr} \overline{B_0}^{\gamma_p^\pm}$  of periodic orbits we notice that after a cyclic permutation under the trace in (5.12) one can employ the fact that  $V_\pm^\dagger V_\pm = \mathbb{1}_2$ , and that  $\text{tr} d_\pm(\mathbf{p}, \mathbf{x}, T_{\gamma_p^\pm}) =: \text{tr} d_{\gamma_p^\pm}$  is independent of  $(\mathbf{p}, \mathbf{x})$ ; hence  $\text{tr} \overline{B_0}^{\gamma_p^\pm} = \text{tr} d_{\gamma_p^\pm}$ . With these identifications the trace formula of [15, 16] is hence recovered.

As a final comment on the trace formula (5.13) let us mention that one can view the left-hand side of (5.13) as resulting from an application of the weighted spectral density

$$d_{\chi, B}(E) := \sum_n \chi(E_n) \langle \psi_n, \hat{B} \psi_n \rangle \delta(E - E_n) \quad (5.16)$$

to the test function  $\rho$  (after a suitable shift of the variable). In this context the trace formula (5.13) can be converted into a distributional identity for the weighted spectral density (5.16),

$$\begin{aligned} d_{\chi, B}(E) = \chi(E) \frac{1}{(2\pi\hbar)^3} \left( \text{vol}(\Omega_E^+) \text{tr} \overline{B_0^+}^E + \text{vol}(\Omega_E^-) \text{tr} \overline{B_0^-}^E \right) + O(\hbar^{-2}) \\ + \chi(E) \frac{1}{2\pi\hbar} \sum_{\gamma_p^\pm} \text{tr} \overline{B_0}^{\gamma_p^\pm} A_{\gamma_p^\pm} e^{\frac{i}{\hbar} S_{\gamma_p^\pm}(E)} (1 + O(\hbar)) . \end{aligned} \quad (5.17)$$

It is in this form that trace formulae are frequently presented (see, e.g., Gutzwiller's original work [1]).

## 6 Semiclassical averages of expectation values

The left-hand side of the trace formula (5.13) can be seen as a weighted superposition of the expectation values  $\langle \psi_n, \hat{B} \psi_n \rangle$  corresponding to the eigenvalues  $E_n$  in some interval about  $E$  of width proportional to  $\hbar$ . This is so since  $\rho \in C^\infty(\mathbb{R})$  is a test function with Fourier transform  $\tilde{\rho} \in C_0^\infty(\mathbb{R}) \subset \mathcal{S}(\mathbb{R})$ . Thus  $\rho$  itself is, indeed, a Schwartz function, i.e. it is rapidly decreasing, and therefore essentially cuts off all terms corresponding to eigenvalues outside of some interval  $[E - \hbar\omega_1, E + \hbar\omega_2]$ . Although the length of this interval shrinks to zero in the semiclassical limit, the number of eigenvalues it contains grows, since according to the Weyl term of the spectral density (compare (5.17) with  $\hat{B} = \mathbb{1}_{\mathcal{H}}$ ) the mean density of eigenvalues increases like  $\hbar^{-3}$ . In the following we therefore want to study a semiclassical average of the expectation values  $\langle \psi_n, \hat{B} \psi_n \rangle$  related to the  $N_I$  eigenvalues  $E_n \in I(E; \hbar) = [E - \hbar\omega, E + \hbar\omega]$ , see (2.6). More precisely, we want to express the limit

$$\lim_{\hbar \rightarrow 0} \frac{1}{N_I} \sum_{E_n \in I(E; \hbar)} \langle \psi_n, \hat{B} \psi_n \rangle \quad (6.1)$$

in terms of classical quantities.

It seems that the trace formula (5.13) is the ideal tool that allows one to achieve the calculation of the limit (6.1). For two reasons, however, the situation is not so straight forward:

1. For the trace formula (5.13) we assumed that all periodic orbits be isolated and non-degenerate. This is a condition which is, e.g., met by hyperbolic classical dynamics. However, hyperbolicity is a strong chaotic property which is not at all necessary for the result we are aiming at. In fact, a considerably weaker condition suffices: it is only required that the points on the energy shells  $\Omega_E^\pm$  that lie on periodic orbits are of Liouville measure zero. Any ergodic dynamical system shares this property, but even many integrable ones as well.
2. For the test function  $\rho$  in the trace formula one cannot simply choose the characteristic function  $\chi_{[-\omega, \omega]}$  of the interval  $[-\omega, \omega]$ , which would provide the sharp cut-off (6.1) in the summation over the eigenvalues, since  $\chi_{[-\omega, \omega]}$  is not smooth and, moreover, its Fourier transform  $\frac{2}{t} \sin \omega t$  is not compactly supported. It even decreases too slowly to make the sum over periodic orbits in (5.13) convergent.

Despite of these objections it is nevertheless possible to calculate the limit (6.1) in rather general situations. For the case of Pauli-Hamiltonians this has, indeed, been carried out in [19]. However, to achieve this one does not employ the trace formula (5.13) directly, but rather starts off from (5.3), which served as the basic relation from which the trace

formula was derived. Again one has to calculate the integral (5.6), but here we are only interested in the leading semiclassical order. By an inspection of the trace formula one realises that this is completely determined by the Weyl term, i.e. by the stationary points  $(\boldsymbol{\xi}_{st}, \boldsymbol{x}_{st}, t_{st})$  with  $t_{st} = 0$  and  $(\boldsymbol{\xi}_{st}, \boldsymbol{x}_{st}) \in \Omega_E^\pm$ . As a non-degeneracy condition we therefore only need that  $E$  is not a critical value for the two Hamiltonians  $H^\pm(\boldsymbol{p}, \boldsymbol{x})$ . For later purposes we, however, require this condition to hold for all  $E' \in [E - \varepsilon, E + \varepsilon]$  with some  $\varepsilon > 0$ . It is then ensured that the non-trivial time components  $t_{st} \neq 0$  of stationary points cannot accumulate at zero (see, e.g., [22]). We stress that no assumptions on the periodic orbits have to be made apart from the condition that they form a measure-zero set on the energy shells. Under the integral (5.6) one now only needs a simple partition of unity,  $1 = h_0(t) + (1 - h_0(t))$ , that separates the stationary points  $(\boldsymbol{\xi}_{st}, \boldsymbol{x}_{st}, 0)$  from those with  $t_{st} \neq 0$ . In order to estimate the latter contribution one exploits the fact that the points on periodic orbits, which are precisely the stationary points  $(\boldsymbol{\xi}_{st}, \boldsymbol{x}_{st})$  with  $t_{st} \neq 0$ , are assumed to be of Liouville measure zero on  $\Omega_E^\pm$ . As a consequence one obtains that the leading semiclassical order is solely determined by the Weyl contribution (see, e.g., [27, 18, 19]), so that

$$\begin{aligned} \sum_n \chi(E_n) \langle \psi_n, \hat{B} \psi_n \rangle \rho\left(\frac{E_n - E}{\hbar}\right) \\ = \chi(E) \frac{\tilde{\rho}(0)}{2\pi} \frac{1}{(2\pi\hbar)^2} \left( \text{vol}(\Omega_E^+) \text{tr } \overline{B_0^+}^E + \text{vol}(\Omega_E^-) \text{tr } \overline{B_0^-}^E \right) + o(\hbar^{-2}) . \end{aligned} \quad (6.2)$$

In a next step one would like to get rid of the test function  $\rho$  and to replace it by a sharp cut-off. Under the conditions mentioned above, which led to the relation (6.2), this can indeed be done with the help of the Tauberian Lemma of [28]. The only point that still has to be clarified is that the Tauberian Lemma requires the expectation values of  $\hat{B}$  to be non-negative. Since, however,  $\hat{B}$  is bounded, this condition can be satisfied after shifting the observable by a suitable constant. In effect, the Tauberian Lemma of [28] then allows to simply replace  $\rho$  by the characteristic function  $\chi_{[-\omega, \omega]}$ , and its Fourier transform by  $\frac{2}{t} \sin \omega t$ . We also recall that  $E$  was chosen to be somewhere inside the gap  $(-mc^2, +mc^2)$  of the essential spectrum of  $\hat{H}$ . Thus, for sufficiently small  $\hbar$  the interval  $I(E; \hbar)$  is completely contained in  $(-mc^2, +mc^2)$  so that the function  $\chi \in C_0^\infty(\mathbb{R})$  that serves as to cut off the essential spectrum can be chosen such that  $\chi(E) = 1 = \chi(E_n)$  for all  $E_n \in I(E; \hbar)$ . Hence

$$\sum_{E_n \in I(E; \hbar)} \langle \psi_n, \hat{B} \psi_n \rangle = \frac{\omega}{\pi} \frac{1}{(2\pi\hbar)^2} \left( \text{vol}(\Omega_E^+) \text{tr } \overline{B_0^+}^E + \text{vol}(\Omega_E^-) \text{tr } \overline{B_0^-}^E \right) + o(\hbar^{-2}) . \quad (6.3)$$

Furthermore, the choice  $\hat{B} = 1_{\mathcal{H}}$  in (6.3) yields a semiclassical representation for the number  $N_I$  of eigenvalues in the interval  $I(E; \hbar)$ ,

$$N_I = \frac{\omega}{\pi} \frac{2}{(2\pi\hbar)^2} \left( \text{vol}(\Omega_E^+) + \text{vol}(\Omega_E^-) \right) + o(\hbar^{-2}) , \quad (6.4)$$

so that (6.3) and (6.4) finally allow to determine the limit (6.1),

$$\lim_{\hbar \rightarrow 0} \frac{1}{N_I} \sum_{E_n \in I(E; \hbar)} \langle \psi_n, \hat{B} \psi_n \rangle = \frac{1}{2} \frac{\text{vol}(\Omega_E^+) \text{tr} \overline{B_0^+}^E + \text{vol}(\Omega_E^-) \text{tr} \overline{B_0^-}^E}{\text{vol}(\Omega_E^+) + \text{vol}(\Omega_E^-)} . \quad (6.5)$$

As desired, the right-hand side of this relation involves only classical quantities.

The result (6.5) can be converted into a statement about averages of the Wigner transforms

$$W[\psi_n](\mathbf{p}, \mathbf{x}) := \int_{\mathbb{R}^3} e^{-\frac{i}{\hbar} \mathbf{p} \cdot \mathbf{y}} \overline{\psi_n}(\mathbf{x} - \frac{1}{2} \mathbf{y}) \otimes \psi_n(\mathbf{x} + \frac{1}{2} \mathbf{y}) \, d\mathbf{y} \quad (6.6)$$

of the eigenspinors  $\psi_n \in I(E; \hbar)$ , since expectation values of Weyl operators can be expressed as

$$\langle \psi_n, \hat{B} \psi_n \rangle = \frac{1}{(2\pi\hbar)^3} \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \text{tr}(W[\psi_n](\mathbf{p}, \mathbf{x}) B(\mathbf{p}, \mathbf{x}; \hbar)) \, d\mathbf{p} \, d\mathbf{x} . \quad (6.7)$$

Here  $\text{tr}(\cdot)$  denotes a matrix trace, whose presence prevents an immediate conclusion from (6.5). To proceed nevertheless, we remark that if one replaces the observable  $\hat{B}$  by its diagonal part  $\hat{B}_d$ , see (3.4) and (3.5), the right-hand side of (6.5) remains unchanged. This immediately follows from the form (3.6) of the principal symbols of the diagonal part and the non-diagonal part, respectively. Thus, in particular,

$$\lim_{\hbar \rightarrow 0} \frac{1}{N_I} \sum_{E_n \in I(E; \hbar)} \langle \psi_n, \hat{B}_{nd} \psi_n \rangle = 0 . \quad (6.8)$$

We can therefore now restrict attention to observables  $\hat{B}$  that are Weyl quantisations of symbols  $B = B_{0,d} = B_0^+ + B_0^-$ . Starting with a quantisation of, e.g.,  $B_0^+$  one splits this matrix valued symbol into a sum of contributions where all matrix entries but one vanish, so that now one essentially deals with scalar operators and symbols. Applying (6.5) to these then finally yields

$$\begin{aligned} & \lim_{\hbar \rightarrow 0} \frac{1}{N_I} \sum_{E_n \in I(E; \hbar)} \frac{1}{(2\pi\hbar)^3} W[\psi_n](\mathbf{p}, \mathbf{x}) \\ &= \frac{1}{2} \frac{\text{vol}(\Omega_E^+) \delta(H^+(\mathbf{p}, \mathbf{x}) - E) P_0^+(\mathbf{p}, \mathbf{x}) + \text{vol}(\Omega_E^-) \delta(H^-(\mathbf{p}, \mathbf{x}) - E) P_0^-(\mathbf{p}, \mathbf{x})}{\text{vol}(\Omega_E^+) + \text{vol}(\Omega_E^-)} . \end{aligned} \quad (6.9)$$

Here the convergence as  $\hbar \rightarrow 0$  has to be understood in the sense of distributions, i.e. after an application to (matrix valued) test functions. In (6.5) the latter are given by the symbols of Weyl operators.

Let us add a few remarks on the result (6.5). Relations of this kind, which express semiclassical averages of quantum observables in terms of classical averages are known as (weak versions of) *Szegő limit formulae* [29]. They are well known for Schrödinger-Hamiltonians (see, e.g., [27]) and have recently been established for Pauli-Hamiltonians



[19]. In the present case the classical side contains the two contributions that arise from projections of the classical observable  $B_0$  to the two eigenspaces of the symbol  $H$  and hence correspond to ‘particles’ and ‘anti-particles’, respectively. The relative weights of the two terms are fixed by the relative volumes of the corresponding energy shells. It often occurs that for a given energy  $E$  only one of the energy shells is non-empty, and then only one contribution appears on the right-hand side of (6.5). The only exceptional situations are those where the Klein paradox occurs, i.e. where a tunneling between particle and anti-particle states is possible. The corresponding mixture is then accounted for by the presence of both terms on the classical side of (6.5). Due to the relation (6.8), however, semiclassically transitions from particle to anti-particle states, or vice versa, play no role. On the right-hand side of (6.9) this effect is caused by the fact that only terms proportional to the projectors  $P_0^\pm$  occur so that the semiclassically averaged Wigner transforms are block-diagonal with respect to the particle and anti-particle subspaces.

Obviously, Szegő limit formulae of the kind (6.5) contain considerably less information on expectation values than trace formulae like (5.13). They demonstrate that the semiclassically leading term of the weighted spectral density (5.17) is the semiclassical average of the observable multiplied by the leading Weyl-term of the spectral density. Fluctuations of expectation values about the semiclassical average are then described by the sum over periodic orbits in (5.17) and therefore depend on classical properties more sensibly than the average itself. However, the trace formula (5.13) does not allow to draw conclusions about individual expectation values since on its spectral side it contains the test function  $\rho$ , whereas on its semiclassical side the Fourier transform  $\tilde{\rho}$  appears. Thus, by Fourier duality, shrinking the (effective) support of  $\rho$  results in a growing (effective) support of  $\tilde{\rho}$ , finally leading to a divergent, and thus uncontrollable, sum over periodic orbits. The smallest support of  $\rho$  that can, indeed, be handled leads to the semiclassical average (6.5). However, in the same way as the Gutzwiller trace formula is not suited for the representation of individual eigenvalues, but enables a semiclassical analysis of spectral correlations (see, e.g., [7, 30]), the trace formula (5.13) can be used to determine correlations of expectation values as, e.g., in [31].

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## References

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